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SPECIFIC CONTACT RESISTANCE AT IN-*n*MoSe$_2$ INTERFACES

C.K SUMESH[a], K.D PATEL[b], V.M PATHAK[b] AND R.SRIVASTAVA[b]

[a]*Department of Physics, Charotar University of Science and Technology – CHANGA ,*
Anand, - 388 421, INDIA
[b]*Department of Physics, Sardar Patel University, Vallabh Vidyanagar, Anand, - 388120, INDIA*

Email: cksumesh.cv@ecchanga.ac.in

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ABSTACT

In this report we discuss the specific contact resistance between molybdenum diselenide single crystals grown by direct vapour transport (DVT) technique with indium deposited contacts. The thermionic emission model was used to find the specific contact resistance. The specific contact resistance was calculated as low as 4.49 x $10^{-9}\Omega$ cm^2. Regardless of being inhomogeneities in the sample thickness due to growth spirals and steps like structure, the spreading resistance of the contact was found to be 5.8 Ω. The measured Hall scattering factor and Hall parameters of indium contacts on MoSe$_2$ evidenced the reliability of the contacts.

I. INTRODUCTION

The performance of any electronic device is determined by a combination of device structure and the material properties of the structure. Metal-semiconductor junctions are essential to any electronic system containing semiconductors. The development of ohmic electrical contacts is an integral stage in the performance of a new material technology. A low contact resistance is the primary requirement for such contacts. They must also be strongly disciple, able to withstand the temperatures, long lasting and finally, they should be compatible with conventional device processing techniques. Ohmic contacts are characterized by measuring the contact resistance arising at the contact-semiconductor junction. Normalizing the contact resistance to the contact area gives rise to the specific contact resistance. For the ideal case a uniform current flow takes place perpendicular to the contact, and in reality, however, the current flow is rarely perpendicular, and the finite resistance of the semiconductor leads to current crowding. The formation of low resistance ohmic contacts to any layered semiconductor is a difficult problem due to the large anisotropic structure and defects during the growth of such semiconductors. Specific contact resistivity (R_c) is the physical parameter that characterizes the quality of a metal-semiconductor contact. As device dimensions shrink, ohmic interfaces with smaller specific contact resistivity are required so that the metal-semiconductor interface resistance be negligible in comparison to the resistances of active devices.

Molybdenum dichalcogenide belongs to the large family of layered transition metal dichalcogenide compounds (TMDC's) [1]. Single crystals of these semiconducting compounds have been receiving increasing attention because of their potential electrochemical and optoelectronic applications [2-5]. With respect to electrochemical and photovoltaic applications single crystals of MoSe$_2$ have been extensively studied. The lowest indirect band gap for MoSe$_2$ was reported to lie between 1.06 and 1.12eV and the lowest direct gap at 1.35eV [6-9]. Due to the combination of the low energy indirect transition (α =

10^4cm^{-1} at 1.45eV) $MoSe_2$ promises to convert solar energy to electrical energy efficiently [10,11]. 2H-$MoSe_2$ layered semiconductors also possess the [12,13] the persistent photoconductivities (PPC) which is an attractive property of solar energy materials.

The anticipations of the theory of contact resistivity regarding the temperature dependence of R_c remain virtually untested in the low R_c regime for $MoSe_2$ type layered materials and is required for the device applications of this material. The present investigation was designed, first, to calculate contact resistance, and second, to investigate the limits that metal-semiconductor contacts impose on device operation at lowered temperatures. Determination of contact resistance necessarily requires the measurement of current and voltage, and where the resistance value is low, involves either a large current density or a small potential difference or both. In order to find the specific contact resistivity (R_c), metal (Ag) semiconductor ($MoSe_2$) junction was prepared. The current transport mechanism of the metal semiconductor contact was then studied in the temperature range of 320K-50K**.**

II. EXPERIMENTAL PROCEDURE

Crystals of $MoSe_2$ were grown by direct vapour transport (DVT) method [14-16] inside a dual zone horizontal furnace. The microstructural examination of as-grown surface of the crystals was accomplished with the help of Axiotech 100 reflected light microscope, Carl Zeiss Jena, Germany. Crystals with flat shining surfaces were chosen with the help of this microscope. These crystals were then washed in acetone to remove contaminations and to make the surface clean. It was kept in the oven for a couple of minutes at 60^0C to dry out the crystals completely. The cleaned crystals were glued onto a suitably cut mica piece. This was then mounted on the substrate holder inside the vacuum chamber. In order to get circular patterns of evaporated metals on the crystal surface the crystals were masked with a thin metal sheet having circular holes of area 3.61 x 10^{-3} cm^2. After reaching the vacuum level of the order of 10^{-6} Torr, pure indium metal ingot were evaporated (5kA^0) from a W-helical boat onto the semiconductor surface. The rate of the evaporation was kept very low to make the deposition uniform over the whole area. The prepared structure was taken out from the chamber. The electrical contacts were taken with low strain thin Ag alloy wires (Lakeshore wire part No.671-260) and Ag paste (Eltec-1228C). This was again mounted inside the vacuum system under a pressure of 10^{-3} Torr for annealing. A slow increase of temperature from room temperature to 100^0C for 10 hours was provided to the crystal. Utmost care was taken during the whole process because $MoSe_2$ crystals are very much soft and brittle. The dc Current – Voltage characteristics were acquired with Keithley 2400 source-measurement unit (SMU) interfaced with a computer and labtracer software. Measurement of current and voltage at various intervals of time with the increment of temperature has been measured to see the effect of heat treatment and the stability of ohmic nature of the contact.

For studying the low temperature stability of the contacts made by above mentioned methods, the sample was mounted on the sample mount stage inside the closed cycle refrigerator (CCR 75014) and contacts were soldered for external circuit. The measurement of resistance over a range of temperatures is made possible with the help of Lakeshore temperature controller (Model 340), which balances the cooling power provided by a closed cycle refrigerator against two heater circuits. The first control loop consists of a temperature sensor and heater attached to the cold end of the refrigerator. The sample is located near the top of the copper sample well and is at a significant distance from the cold end. A temperature sensor mounted directly to the sample provides a much more accurate measure of the actual sample temperature. When the variables were set correctly, temperature was also set constant at the desired value using Lakeshore temperature controller and closed cycle cryostat. After stabilizing the set temperature, measurements were started and the resistance measured between the pair of contacts and the data were stored as spreadsheet in the computer memory. The experiment was performed between temperatures 320-50K. The Hall parameters were extracted by Hall effect measurement system model 7504 supplied by Lakeshore Cryotronics, Inc., USA.

III. RESULT AND DISCUSSION

The freshly prepared ohmic contacts with conventional method of evaporated indium shows a highly non ohmic behavior and shows a contact resistance of 50kΩ. After 12 hours of continuous annealing at 100^0C the contact resistance found to be around 22kΩ and it was seen to saturated around this value with further annealing under the same condition. The high value of resistance could be attributed to the inhomogeneous deposition of indium over the terminated layered growth of the semiconductor along with poor adhesion of Ag paste bonded with the contact.

The variation of I-V characteristics of In-MoSe$_2$ contact is shown in figure 1. The observed significant decrease in contact resistance magnitude of around 75 percent can be attributed to (i) the diffusion of indium in to the layers of the crystal and (ii) curing of Ag paste with heat treatment. However further annealing at higher temperature of about 150^{0}C, the contact resistance increases, which may be due to the evaporation of indium from the surface of MoSe$_2$.

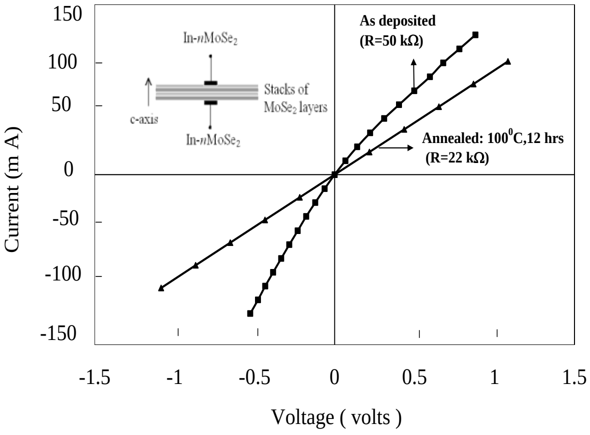

FIGURE 1. I-V characteristics of In-MoSe$_2$ contact.

In order to see the dominant charge transport mechanism characteristic, energy related to the tunneling probability (E$_{00}$) for MoSe$_2$ was compared with kT/q. The value of E$_{00}$ was calculated from the equation 1 [17].

$$E_{00} = \frac{1}{2}\hbar q\left[\frac{N_D}{m^*\varepsilon}\right]^{\frac{1}{2}} \qquad (1)$$

where m* is the effective mass of electrons in the semiconductor, ε is the permittivity and N$_D$ is the donor concentration. The values of m* and ε have been used from the references [18,19]. The relation for donor concentration N$_D$ with temperature is expressed as [20]

$$n_d = N_D\left[1\Big/1+\beta\exp(E_d - E_F)/k_BT\right] \qquad (2)$$

where, n$_d$ is the density of electrons on donor atom, β donor degeneracy, E$_d$ donor energy level, E$_F$ Fermi energy, k$_B$ Boltzmann constant and T absolute temperature.

Assuming uniform doping concentration N$_D$, complete depletion of the space charge region and ignoring image force lowering where E$_{00}$ << kT, carriers are thermionically emitted over the barriers. Therefore thermionic emission (TE) conduction mechanism has been identified as the dominant charge transport mechanism [17]. The thermionic emission theory assumes that the current is controlled only by the transfer of carriers across the top of the barrier; provided they move towards the barrier and the drift and diffusion that occur as a result of collisions within the space charge region are considered unimportant. The actual shape of the barrier is hereby ignored.

Since N$_D$ is a temperature dependent parameter, the value of E$_{00}$ was calculated for all the N$_D$ values. The variation of E$_{00}$ for different values of N$_D$ is plotted in figure 2. Result shows that $kT\big/E_{00} >> 1$ for a temperature range 50 < T < 320 K [21].

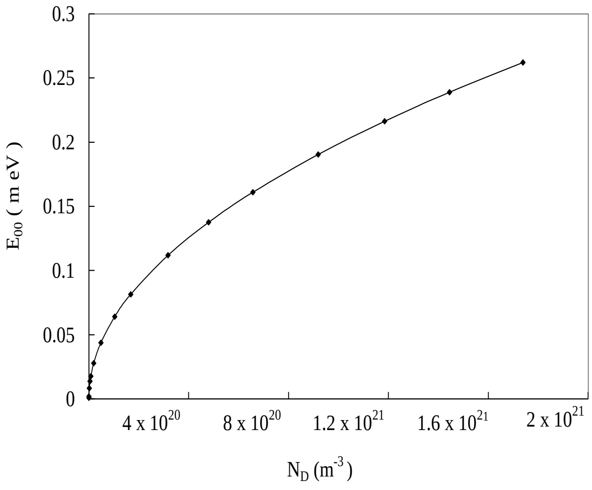

FIGURE 2. Variation of E$_{00}$ as a function of change in N$_D$.

As E$_{00}$ increases with N$_D$, the barrier for the tunneling process becomes thinner, and in turn results in increased tunneling of carriers, For low to moderate doping levels and kT >> E$_{00}$, from the standard thermionic emission expression the specific contact resistance (R$_c$) is given by

$$R_c = \frac{k_B}{A^{**}qT}\exp\left(\frac{q\phi_B}{k_BT}\right) \qquad (3)$$

where A** is the effective Richardson constant which is equal to $4\pi q m_e^* k_B^2\big/h^3$ for n type semiconductors, Φ$_B$ is barrier height, T is temperature and k$_B$ is Boltzmann constant. The Richardson constant was calculated to be 60 Acm^{-2}K^{-2}. The value of specific contact resistance was calculated according to the equation (3) at various temperatures ranging from 320-50K. The specific contact resistance at the metal - semiconductor interface is known to be a monotonically decreasing as a function of temperature. This variation of specific contact resistance with temperature of In-$MoSe_2$ contact is plotted in figure (3). The value of R_c at room temperature is found to be 4.49 x $10^{-9}\Omega$ cm^2. The inverse nature of the specific contact resistivity R_c with temperature according to equation 2 could be attributed to a residual barrier between metallization and semiconductor, entailing a strong contribution of thermionic emission current through the contact.

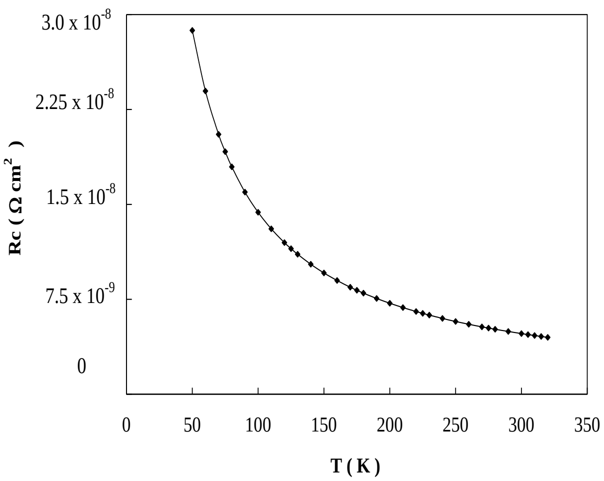

FIGURE 3. Specific contact resistance plot for indium contact at various temperatures.

The spreading resistance of a circular contact on a semiconductor is also an important quantity in many semiconductor device measurements and device design. In order to find the spreading resistance the finite element method has been used according to the formula [22],

$$R_s = \frac{\rho}{r}\begin{pmatrix} 0.31844h - 0.28374h^2 + \\ 0.21145h^3 - 0.17193h^4 + \\ 0.10657h^5 \end{pmatrix} \qquad (4)$$

Where, r is contact radius, ρ is resistivity and h is ratio of substrate thickness to contact radius. The value thus obtained was 5.8 Ω. The components of the contact resistance could be divided into two parts such as the Schottky diode and the spreading resistance caused by current crowding that is due to the small size of the contact. The non-linear behavior is generally caused by spreading resistance. The value of R_s is very much negligible in our case.

In order to validate the surety of the contacts made by indium, Hall effect experiment has been performed using van der Pauw (vdP) resistivity method. A good Hall sample is characterized by its I-V characteristics obtained between two contacts amongst a set of four contacts prepared in van der Pauw geometry on four corners along its periphery. If this characteristic are found linear over a range of current change and they are close by, then the sample is considered suitable for further Hall measurements. The vdP factor is about 0.999 (nearly 1) for almost all temperature ranges. The Hall scattering factor calculated from the temperature dependent Hall coefficient and carrier density is found to be 0.97 to1 which is the immediate requirement for extracting the electrical transport properties of semiconducting materials. In spite of being inhomogeneities in the sample thickness due to growth spirals and steps like structure the indium contacts in vdP geometry provides reliable Hall effect measurements. The value of vdP factor depends on the metallization methods to $MoSe_2$ crystals and the Hall parameters are strongly influenced by the vdP factor.

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Ohmic metallization	Resistivity (Ω-cm)	Density (1/cm³)	Mobility (cm²/V s)
Indium	2.2	4.54 x10^{17}	76
Reported			
1. [3]	0.47	1.3 x10^{17}	126.0
2. [23]	25	3.5 x10^{16}	31.4
3. [24]	1	1.6 x10^{17}	40.0
4. [25]	11.5	1.8 x10^{16}	30.30
5. [26]	1.5	5.0 x10^{16}	100.0

Table 1. Observed and reported Hall parameters of $MoSe_2$ crystals at 300K

IV. CONCLUSION

Electrical characteristics of Ohmic contact on n-$MoSe_2$ semiconductor substrates with indium metal were studied. The as prepared Ohmic contacts where not perfectly symmetric but the contact resistance improved after annealing. The specific contact resistivity as low as $4.49 \times 10^{-9}\ \Omega\ cm^2$ was obtained at room temperature. This method provides a useful way of making ohmic contacts on layered dichalcogenides. The spreading resistance of the contact was found to be 5.8 Ω. The electrical characterization shows good values which may support the device performance for these types of materials.

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